



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 4KO0 / pdb_00004ko0
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
COMPLEX WITH an anilinympyrimidine derivative (JLJ-135)
Authors : Das, K.; Bauman, J.D.; Arnold, E.
Deposited on : 2013-05-10
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

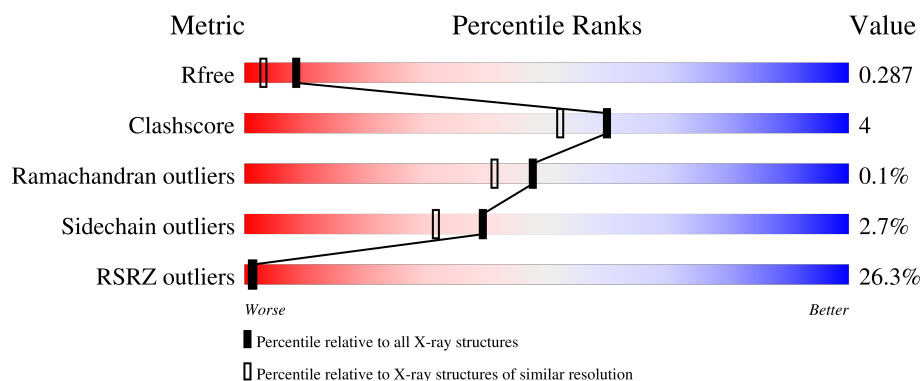
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	26% 88% 10% .
2	B	428	25% 85% 10% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8309 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 reverse transcriptase, p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	2	0
			4521	2926	751	836	8			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	172	ALA	LYS	engineered mutation	UNP P03366
A	173	ALA	LYS	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

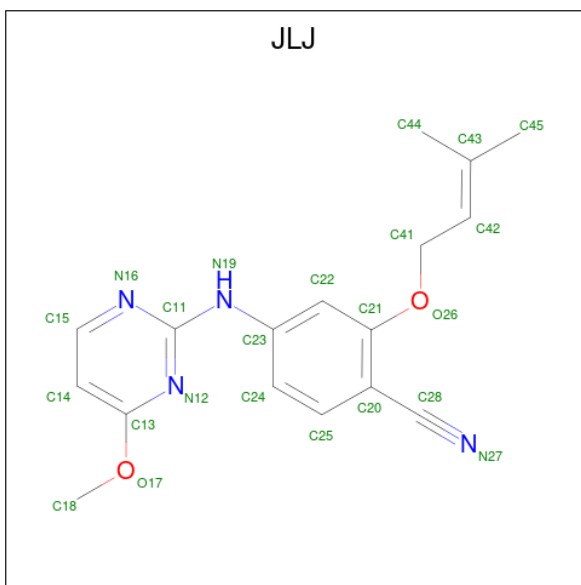
- Molecule 2 is a protein called HIV-1 reverse transcriptase, p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	410	Total	C	N	O	S	0	2	0
			3409	2221	564	617	7			

There is a discrepancy between the modelled and reference sequences:

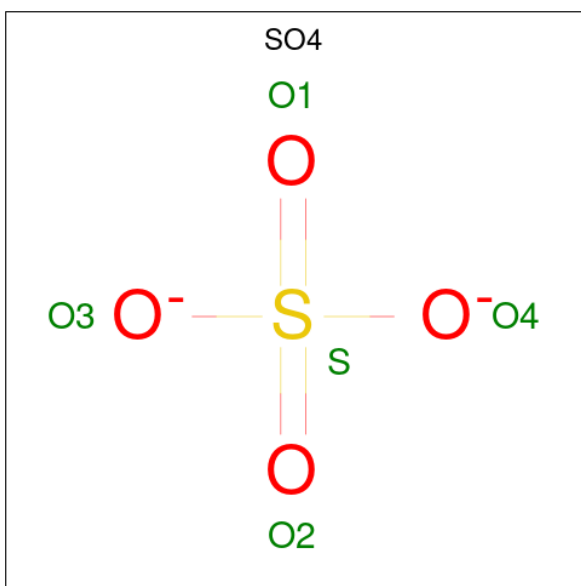
Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 4-[(4-methoxypyrimidin-2-yl)amino]-2-[(3-methylbut-2-en-1-yl)oxy]benzonitrile (CCD ID: JLJ) (formula: C₁₇H₁₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

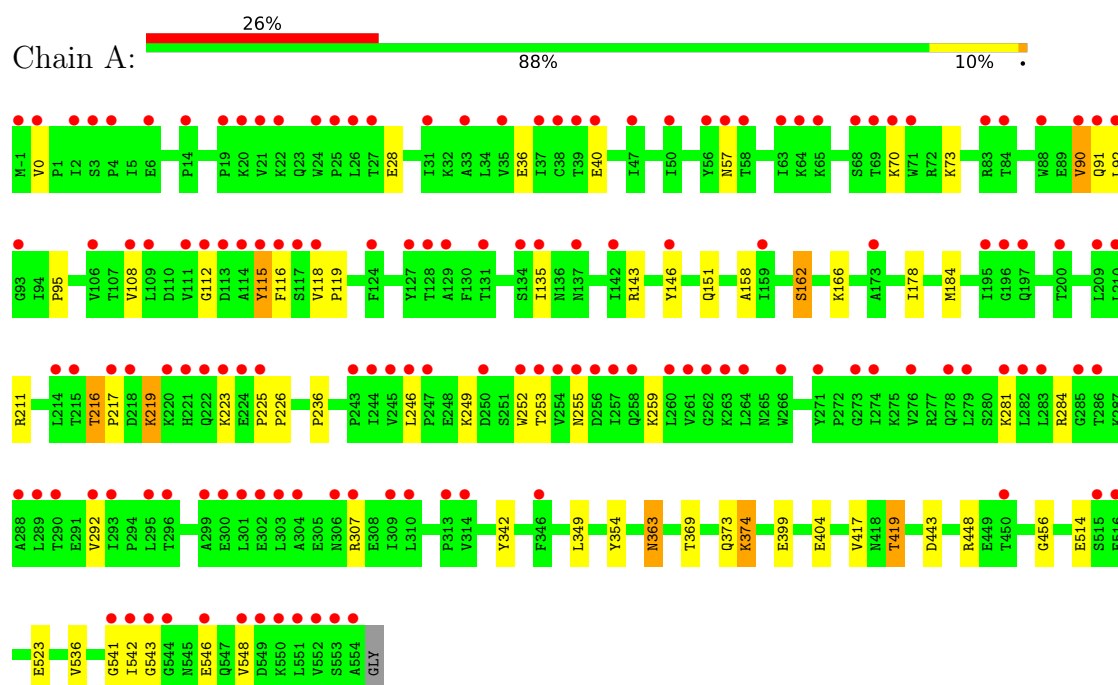
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		
6	B	148	Total	O	0	0
			148	148		

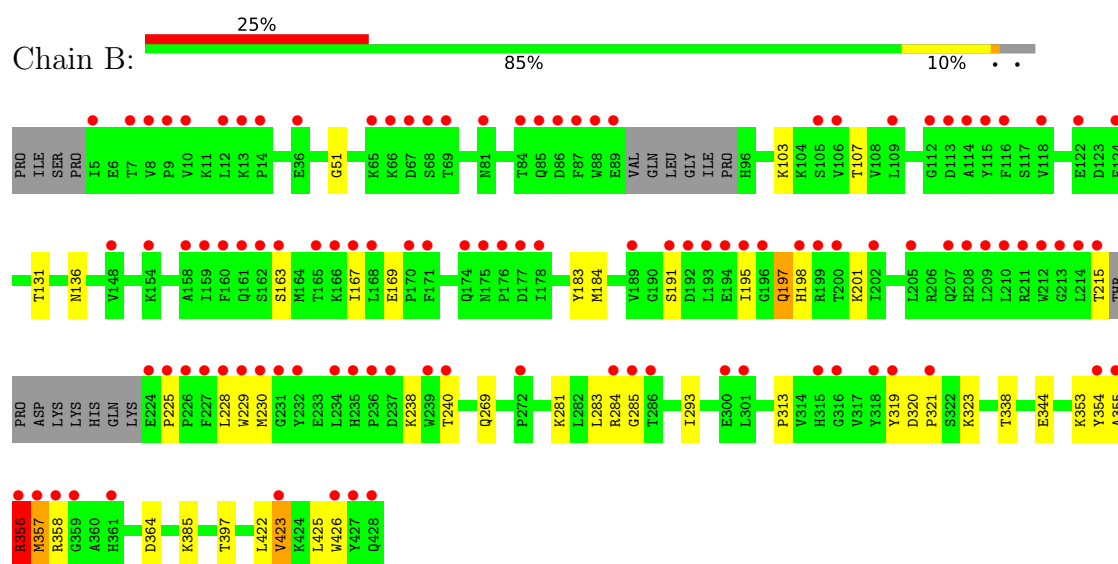
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HIV-1 reverse transcriptase, p66 subunit



- Molecule 2: HIV-1 reverse transcriptase, p51 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.21Å 73.95Å 109.20Å 90.00° 100.23° 90.00°	Depositor
Resolution (Å)	29.31 – 1.95 29.31 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.31-1.95) 98.7 (29.31-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.237 , 0.275 (Not available) , 0.287	Depositor DCC
R_{free} test set	1863 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8309	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, JLJ, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/4643	0.84	6/6311 (0.1%)
2	B	0.50	0/3511	0.85	9/4768 (0.2%)
All	All	0.53	0/8154	0.84	15/11079 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	THR	CA-C-N	-7.26	117.66	122.60
2	B	131	THR	C-N-CA	-7.26	117.66	122.60
1	A	419	THR	CA-C-N	6.26	124.23	119.66
1	A	419	THR	C-N-CA	6.26	124.23	119.66
2	B	51	GLY	CA-C-N	6.02	125.72	119.82
2	B	51	GLY	C-N-CA	6.02	125.72	119.82
1	A	223	LYS	N-CA-C	5.77	118.95	109.72
1	A	90	VAL	N-CA-C	5.66	116.30	110.36
1	A	456	GLY	N-CA-C	5.46	118.56	110.42
2	B	293	ILE	CB-CA-C	-5.43	104.61	110.85
1	A	541	GLY	N-CA-C	-5.38	107.79	115.64
2	B	240	THR	N-CA-C	-5.27	105.19	111.03
2	B	423	VAL	N-CA-C	5.11	119.19	112.04
2	B	356	ARG	N-CA-C	5.07	117.22	109.62
2	B	364	ASP	CB-CA-C	-5.05	102.73	110.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4521	0	4576	40	0
2	B	3409	0	3427	34	0
3	A	23	0	18	2	0
4	A	10	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	A	190	0	0	3	0
6	B	148	0	0	2	0
All	All	8309	0	8033	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:ARG:H	2:B:356:ARG:HD2	1.17	1.08
1:A:543:GLY:HA3	2:B:285:GLY:H	1.43	0.82
2:B:356:ARG:HD2	2:B:356:ARG:N	1.98	0.79
2:B:355:ALA:H	2:B:356:ARG:HD2	1.51	0.76
2:B:320:ASP:HB3	2:B:323:LYS:HE2	1.76	0.68
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.76	0.67
2:B:356:ARG:H	2:B:356:ARG:CD	1.98	0.67
2:B:323:LYS:O	2:B:385:LYS:NZ	2.29	0.66
1:A:404:GLU:HG3	6:A:849:HOH:O	1.96	0.65
1:A:373[A]:GLN:NE2	2:B:397:THR:OG1	2.28	0.65
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.30	0.64
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.81	0.62
1:A:28:GLU:HG3	1:A:135:ILE:HD12	1.82	0.59
1:A:216:THR:OG1	1:A:217:PRO:HD2	2.03	0.59
1:A:543:GLY:HA2	1:A:546:GLU:HB3	1.86	0.58
1:A:543:GLY:HA3	2:B:285:GLY:N	2.18	0.57
2:B:356:ARG:O	2:B:357:MET:HE3	2.04	0.56
1:A:354:TYR:HD1	1:A:374:LYS:HE2	1.70	0.56
1:A:116:PHE:HE1	1:A:151:GLN:HE21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:O	1:A:40:GLU:HG2	2.09	0.53
1:A:543:GLY:N	2:B:283:LEU:O	2.42	0.52
2:B:319:TYR:OH	2:B:385:LYS:HE2	2.11	0.50
1:A:281:LYS:HE3	1:A:284:ARG:NH2	2.27	0.50
2:B:358:ARG:O	2:B:358:ARG:HG2	2.11	0.50
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.44	0.49
2:B:313:PRO:O	6:B:696:HOH:O	2.20	0.49
2:B:163:SER:O	2:B:167:ILE:HG13	2.13	0.49
1:A:523:GLU:OE1	6:A:868:HOH:O	2.20	0.48
1:A:363:ASN:OD1	1:A:363:ASN:C	2.56	0.48
1:A:225:PRO:HA	1:A:226:PRO:C	2.38	0.48
2:B:191:SER:HG	2:B:198:HIS:CE1	2.27	0.48
2:B:225:PRO:HG3	2:B:228:LEU:HD23	1.97	0.47
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.49	0.47
3:A:601:JLJ:N12	3:A:601:JLJ:H7	2.30	0.46
1:A:184:MET:O	6:A:873:HOH:O	2.20	0.46
2:B:354:TYR:HA	2:B:356:ARG:HH11	1.81	0.46
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.97	0.46
1:A:90:VAL:O	1:A:92:LEU:N	2.49	0.45
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.51	0.45
1:A:255:ASN:O	1:A:259:LYS:HG3	2.17	0.45
1:A:342:TYR:HA	1:A:349:LEU:HD13	1.97	0.45
1:A:543:GLY:HA3	2:B:284:ARG:HA	1.99	0.45
2:B:269:GLN:NE2	6:B:675:HOH:O	2.24	0.45
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.52	0.44
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.00	0.44
2:B:358:ARG:O	2:B:358:ARG:CG	2.65	0.44
2:B:195:ILE:HA	2:B:198:HIS:HB3	1.99	0.44
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.83	0.44
2:B:107:THR:OG1	2:B:198:HIS:NE2	2.42	0.44
1:A:95:PRO:HA	2:B:136:ASN:O	2.17	0.43
1:A:216:THR:OG1	1:A:217:PRO:CD	2.65	0.43
1:A:369:THR:O	1:A:373[B]:GLN:HG2	2.18	0.43
1:A:536:VAL:HB	1:A:542:ILE:HD13	2.00	0.43
2:B:229:TRP:CH2	2:B:230:MET:HE3	2.52	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	2.00	0.43
2:B:338:THR:HG22	2:B:353:LYS:HG3	2.01	0.43
1:A:236:PRO:HA	3:A:601:JLJ:H9	2.00	0.42
2:B:320:ASP:HA	2:B:321:PRO:HD2	1.85	0.42
1:A:70:LYS:HE3	1:A:70:LYS:HB2	1.94	0.41
2:B:197:GLN:O	2:B:201:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LYS:HD3	2:B:103:LYS:HA	1.88	0.41
1:A:542:ILE:HG12	2:B:283:LEU:HD12	2.01	0.41
1:A:112:GLY:O	1:A:115:TYR:HB2	2.21	0.41
1:A:158:ALA:O	1:A:162:SER:OG	2.34	0.41
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.56	0.41
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.31	0.40
2:B:355:ALA:N	2:B:356:ARG:HD2	2.25	0.40
1:A:90:VAL:C	1:A:92:LEU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/557 (100%)	543 (98%)	11 (2%)	1 (0%)	43	36
2	B	406/428 (95%)	391 (96%)	15 (4%)	0	100	100
All	All	961/985 (98%)	934 (97%)	26 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	496/495 (100%)	482 (97%)	14 (3%)	38	30
2	B	374/390 (96%)	365 (98%)	9 (2%)	43	36
All	All	870/885 (98%)	847 (97%)	23 (3%)	39	33

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	108	VAL
1	A	115	TYR
1	A	162	SER
1	A	166	LYS
1	A	178	ILE
1	A	211[B]	ARG
1	A	216	THR
1	A	219	LYS
1	A	363	ASN
1	A	374	LYS
1	A	399	GLU
1	A	448	ARG
1	A	514	GLU
2	B	169	GLU
2	B	197	GLN
2	B	215	THR
2	B	238	LYS
2	B	281	LYS
2	B	356	ARG
2	B	357	MET
2	B	422	LEU
2	B	425	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	258	GLN
1	A	278	GLN
1	A	509	GLN

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	524	GLN
2	B	151	GLN
2	B	161	GLN
2	B	207	GLN
2	B	269	GLN
2	B	336	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	A	604	-	3,3,3	0.41	0	2,2,2	0.80	0
3	JLJ	A	601	-	24,24,24	1.46	2 (8%)	31,31,31	2.55	8 (25%)
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.29	0
4	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.11	0
5	EDO	B	501	-	3,3,3	0.19	0	2,2,2	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	604	-	-	1/1/1/1	-
3	JLJ	A	601	-	-	2/14/14/14	0/2/2/2
5	EDO	B	501	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	JLJ	C20-C28	4.69	1.51	1.44
3	A	601	JLJ	O26-C21	3.12	1.43	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	JLJ	O26-C41-C42	6.52	120.98	107.96
3	A	601	JLJ	C15-N16-C11	6.51	120.86	115.42
3	A	601	JLJ	N16-C11-N12	-5.95	120.67	126.42
3	A	601	JLJ	C11-N12-C13	5.09	120.81	115.00
3	A	601	JLJ	C14-C15-N16	-3.17	120.09	123.97
3	A	601	JLJ	C15-C14-C13	2.96	117.25	115.48
3	A	601	JLJ	C41-C42-C43	-2.91	122.06	126.76
3	A	601	JLJ	O17-C13-C14	2.04	120.38	116.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

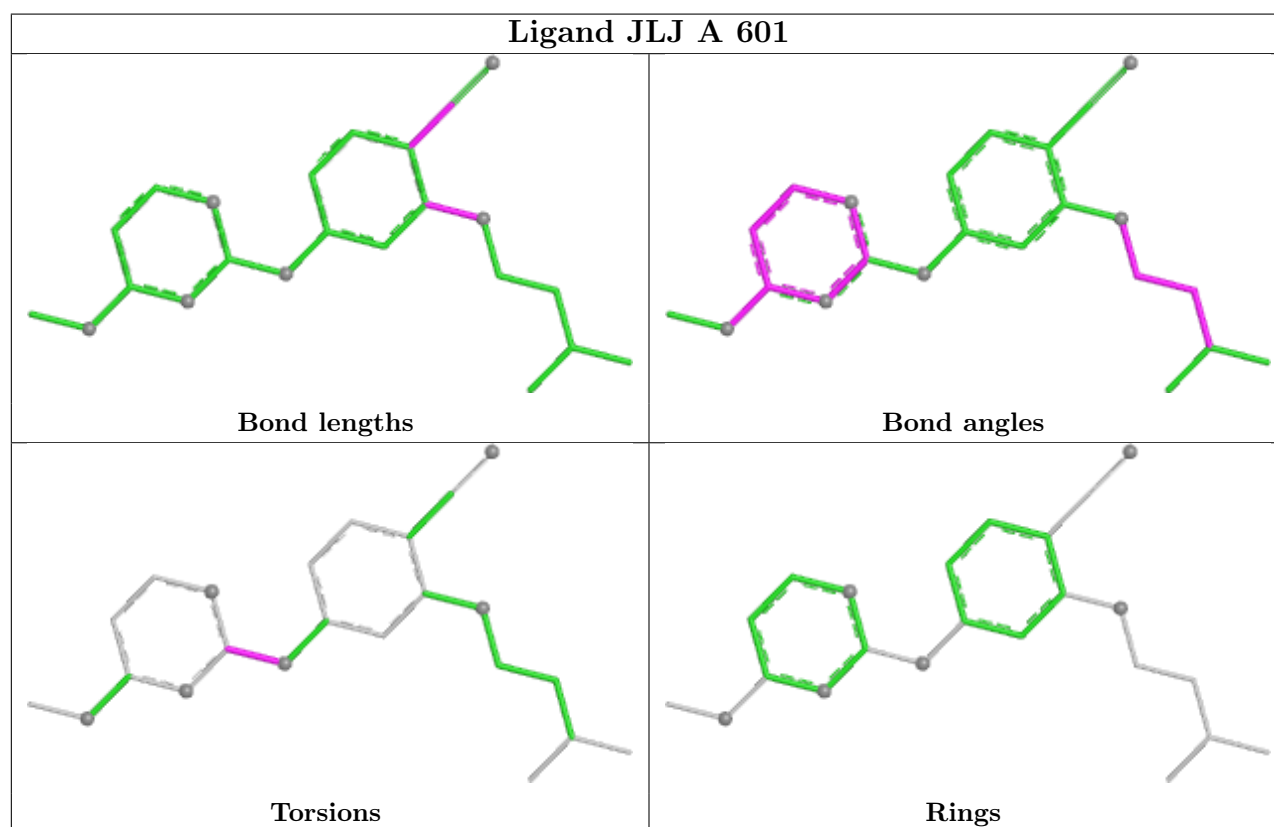
Mol	Chain	Res	Type	Atoms
5	B	501	EDO	O1-C1-C2-O2
3	A	601	JLJ	N12-C11-N19-C23
5	A	604	EDO	O1-C1-C2-O2
3	A	601	JLJ	N16-C11-N19-C23

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	JLJ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	556/557 (99%)	1.33	145 (26%)  	22, 53, 93, 124	1 (0%)
2	B	410/428 (95%)	1.41	109 (26%)  	20, 51, 101, 120	2 (0%)
All	All	966/985 (98%)	1.36	254 (26%)  	20, 52, 99, 124	3 (0%)

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	LEU	7.0
2	B	212	TRP	6.3
2	B	209	LEU	6.1
2	B	240	THR	6.0
2	B	5	ILE	6.0
2	B	214	LEU	5.9
2	B	193	LEU	5.9
1	A	40	GLU	5.8
1	A	24	TRP	5.6
2	B	195	ILE	5.6
2	B	355	ALA	5.4
2	B	225	PRO	5.4
1	A	253	THR	5.2
2	B	88	TRP	5.0
1	A	290	THR	4.9
2	B	232	TYR	4.8
1	A	113	ASP	4.7
1	A	90	VAL	4.7
2	B	7	THR	4.7
2	B	69	THR	4.7
1	A	261	VAL	4.7
1	A	256	ASP	4.6
1	A	116	PHE	4.6
1	A	552	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	246	LEU	4.5
2	B	354	TYR	4.5
1	A	301	LEU	4.5
1	A	279	LEU	4.4
2	B	239	TRP	4.3
1	A	288	ALA	4.3
2	B	356	ARG	4.3
1	A	551	LEU	4.3
1	A	254	VAL	4.3
2	B	229	TRP	4.3
2	B	202	ILE	4.2
1	A	221	HIS	4.2
2	B	234	LEU	4.2
1	A	214	LEU	4.1
1	A	543	GLY	4.1
2	B	284	ARG	4.0
1	A	302	GLU	4.0
1	A	252	TRP	4.0
1	A	292	VAL	4.0
1	A	255	ASN	3.9
2	B	227	PHE	3.9
1	A	541	GLY	3.9
1	A	544	GLY	3.9
1	A	92	LEU	3.9
2	B	198	HIS	3.9
2	B	428	GLN	3.9
1	A	247	PRO	3.9
1	A	129	ALA	3.8
2	B	196	GLY	3.8
2	B	105	SER	3.8
2	B	228	LEU	3.8
2	B	357	MET	3.8
2	B	10	VAL	3.8
1	A	131	THR	3.8
1	A	33	ALA	3.8
1	A	257	ILE	3.8
1	A	210	LEU	3.7
2	B	215	THR	3.7
2	B	427	TYR	3.7
1	A	554	ALA	3.7
2	B	230	MET	3.7
1	A	69	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	213	GLY	3.6
1	A	282	LEU	3.6
1	A	38	CYS	3.6
1	A	262	GLY	3.6
2	B	235	HIS	3.6
1	A	-1	MET	3.5
1	A	309	ILE	3.5
1	A	258	GLN	3.5
2	B	160	PHE	3.5
1	A	68	SER	3.5
2	B	66	LYS	3.5
1	A	115	TYR	3.5
1	A	127	TYR	3.5
2	B	194	GLU	3.5
2	B	159	ILE	3.5
1	A	4	PRO	3.4
1	A	200	THR	3.4
2	B	318	TYR	3.4
1	A	112	GLY	3.4
1	A	273	GLY	3.4
2	B	87	PHE	3.4
2	B	178	ILE	3.4
1	A	546	GLU	3.4
1	A	39	THR	3.4
2	B	86	ASP	3.4
1	A	299	ALA	3.4
2	B	148	VAL	3.3
1	A	70	LYS	3.3
1	A	295	LEU	3.2
1	A	245	VAL	3.2
2	B	114	ALA	3.2
1	A	243	PRO	3.2
2	B	8	VAL	3.2
2	B	162	SER	3.2
2	B	68	SER	3.1
1	A	306	ASN	3.1
1	A	91	GLN	3.1
1	A	286	THR	3.1
2	B	9	PRO	3.1
2	B	176	PRO	3.1
2	B	174	GLN	3.1
2	B	163	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	65	LYS	3.0
2	B	426	TRP	3.0
1	A	19	PRO	3.0
1	A	304	ALA	3.0
2	B	167	ILE	3.0
2	B	106	VAL	2.9
1	A	64	LYS	2.9
1	A	0	VAL	2.9
2	B	165	THR	2.9
1	A	223	LYS	2.9
1	A	57	ASN	2.8
2	B	158	ALA	2.8
2	B	122	GLU	2.8
1	A	285	GLY	2.8
2	B	189	VAL	2.8
1	A	224	GLU	2.8
1	A	293	ILE	2.8
2	B	84	THR	2.8
2	B	171	PHE	2.8
1	A	281	LYS	2.8
2	B	109	LEU	2.8
1	A	314	VAL	2.8
1	A	146	TYR	2.7
2	B	175	ASN	2.7
1	A	549	ASP	2.7
1	A	225	PRO	2.7
1	A	260	LEU	2.7
1	A	195	ILE	2.7
1	A	307	ARG	2.7
1	A	550	LYS	2.7
1	A	21	VAL	2.7
2	B	285	GLY	2.7
1	A	6	GLU	2.7
1	A	250	ASP	2.6
1	A	71	TRP	2.6
1	A	25	PRO	2.6
1	A	26	LEU	2.6
2	B	168	LEU	2.6
1	A	274	ILE	2.6
1	A	114	ALA	2.6
2	B	211	ARG	2.6
1	A	263	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	200	THR	2.6
2	B	170	PRO	2.6
2	B	272	PRO	2.6
1	A	303	LEU	2.6
2	B	205	LEU	2.6
1	A	35	VAL	2.6
1	A	264	LEU	2.6
1	A	31	ILE	2.6
1	A	542	ILE	2.6
2	B	13	LYS	2.6
1	A	296	THR	2.6
2	B	286	THR	2.6
1	A	271	TYR	2.5
2	B	210	LEU	2.5
1	A	2	ILE	2.5
1	A	218	ASP	2.5
2	B	115	TYR	2.5
1	A	142	ILE	2.5
1	A	553	SER	2.5
2	B	14	PRO	2.5
2	B	112	GLY	2.4
1	A	300	GLU	2.4
1	A	88	TRP	2.4
1	A	222	GLN	2.4
1	A	3	SER	2.4
1	A	109	LEU	2.4
1	A	47	ILE	2.4
2	B	315[A]	HIS	2.4
2	B	154	LYS	2.4
1	A	50	ILE	2.4
1	A	83	ARG	2.4
2	B	89	GLU	2.4
1	A	14	PRO	2.4
2	B	161	GLN	2.4
1	A	118	VAL	2.4
2	B	423	VAL	2.4
2	B	12	LEU	2.3
1	A	244	ILE	2.3
1	A	56	TYR	2.3
2	B	116	PHE	2.3
1	A	37	ILE	2.3
2	B	199	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	224	GLU	2.3
1	A	278	GLN	2.3
1	A	450	THR	2.3
2	B	321	PRO	2.3
2	B	231	GLY	2.3
2	B	359	GLY	2.3
1	A	515	SER	2.3
1	A	111	VAL	2.3
1	A	548	VAL	2.3
1	A	346	PHE	2.2
2	B	236	PRO	2.2
1	A	117	SER	2.2
2	B	67	ASP	2.2
1	A	106	VAL	2.2
1	A	137	ASN	2.2
2	B	208	HIS	2.2
1	A	20	LYS	2.2
1	A	22	LYS	2.2
1	A	220	LYS	2.2
2	B	166	LYS	2.2
1	A	128	THR	2.2
1	A	215	THR	2.2
1	A	173	ALA	2.2
2	B	177	ASP	2.2
1	A	108	VAL	2.2
1	A	197	GLN	2.2
2	B	85	GLN	2.2
1	A	276	VAL	2.2
1	A	58	THR	2.2
2	B	226	PRO	2.2
2	B	358	ARG	2.2
1	A	135	ILE	2.1
2	B	191	SER	2.1
1	A	196	GLY	2.1
1	A	209	LEU	2.1
1	A	283	LEU	2.1
2	B	301	LEU	2.1
2	B	124	PHE	2.1
2	B	192	ASP	2.1
1	A	84	THR	2.1
2	B	65	LYS	2.1
1	A	217	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	124	PHE	2.1
1	A	63	ILE	2.1
2	B	237	ASP	2.1
1	A	134	SER	2.1
1	A	516	GLU	2.1
2	B	36	GLU	2.1
1	A	93	GLY	2.1
2	B	81	ASN	2.1
1	A	313	PRO	2.1
1	A	310	LEU	2.1
1	A	159	ILE	2.0
2	B	300	GLU	2.0
2	B	207	GLN	2.0
2	B	118	VAL	2.0
1	A	266	TRP	2.0
2	B	113	ASP	2.0
2	B	361	HIS	2.0
1	A	27	THR	2.0
2	B	316	GLY	2.0
2	B	319	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

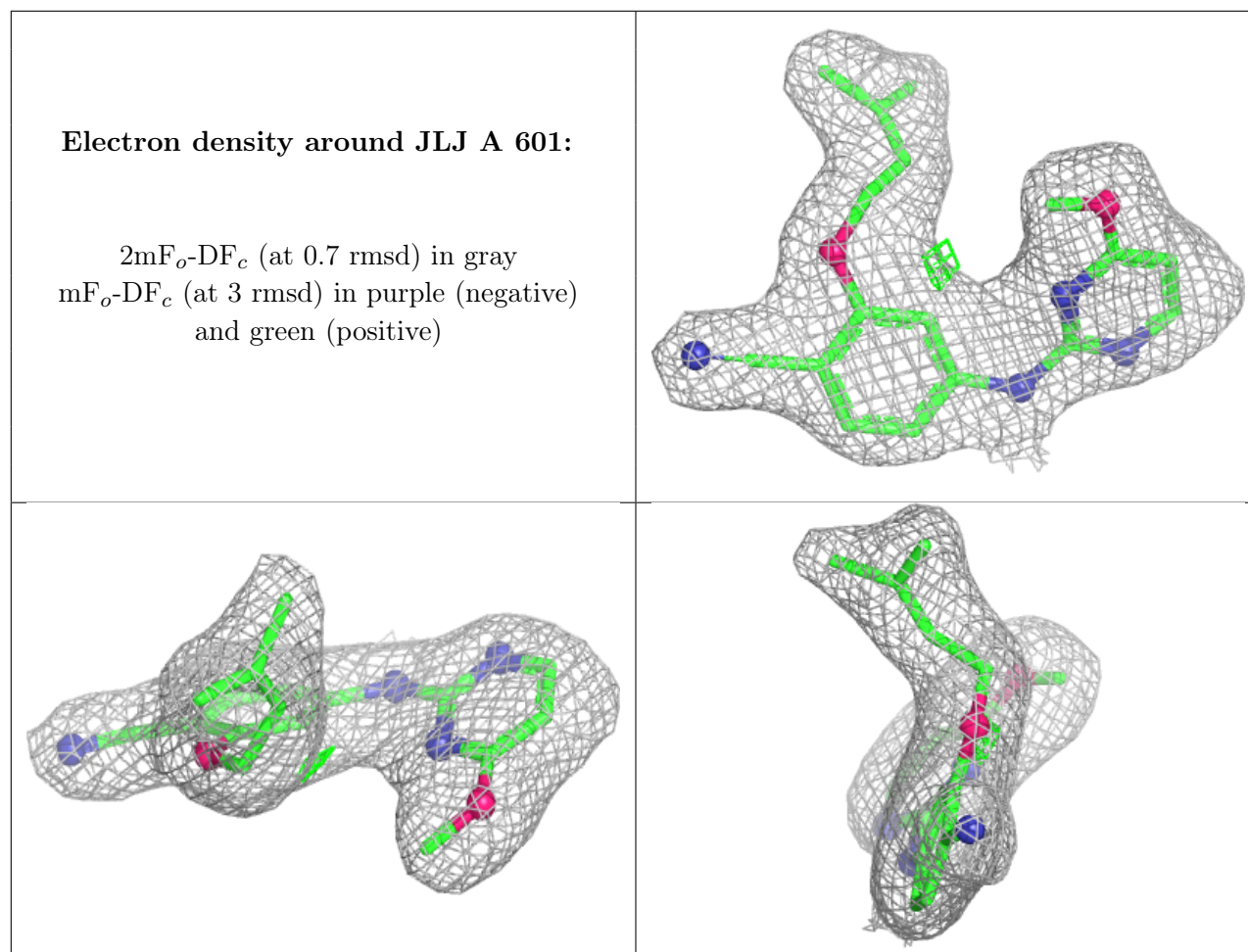
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	603	5/5	0.64	0.13	68,68,90,91	0
4	SO4	A	602	5/5	0.82	0.10	70,74,79,85	0
5	EDO	A	604	4/4	0.93	0.11	41,43,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	501	4/4	0.93	0.11	40,42,45,46	0
3	JLJ	A	601	23/23	0.94	0.09	35,40,46,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.